

An investigation of internal rotations and analysis of vibrational spectra of dichloroacetyl isocyanate. Badawi, H. M.; Forner, W.; Oloriegbe, Y. S

Abstract

The conformational stability and vibrational IR and Raman spectra of dichloroacetyl isocyanate ($\text{CHCl}_2\text{CONCO}$) were investigated by ab initio MP2 and d. functional B3LYP calcns. using the 6-311++G** basis set. From the potential energy scans of the internal rotations in both the halomethyl and the isocyanate rotors, the mol. was predicted to exist in the cis-cis .tautm. cis-trans conformational equil. The cis-cis (the hydrogen atom of the CHCl_2 group and the NCO group, both eclipse the carbonyl C:O bond) form was predicted to be the predominant conformation at ambient temp. Vibrational wavenumbers were computed for the mol. at DFT-B3LYP/6-311++G** level. Normal coordinate calcns. were carried out to obtain the potential energy distributions among the symmetry coordinates of the normal modes for the mol. The theor. vibrational assignments were compared with exptl. ones and the ratio of obsd. to calcd. wavenumbers of about 0.97-1.04 was obtained.